



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:45 AM UTC

PDB ID : 4H31 / pdb_00004h31
Title : Crystal structure of anabolic ornithine carbamoyltransferase from *Vibrio vulnificus* in complex with carbamoyl phosphate and L-norvaline
Authors : Shabalin, I.G.; Winsor, J.; Grimshaw, S.; Osinski, T.; Chordia, M.D.; Shuvalova, L.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-09-13
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

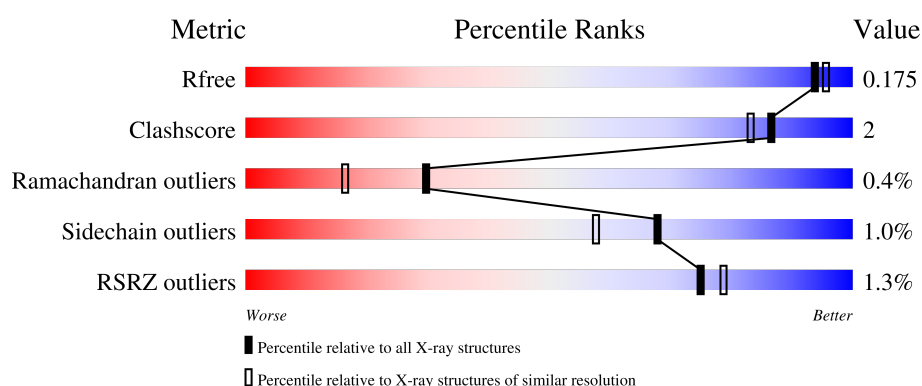
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	358	% 88% 5% 6%
1	B	358	% 89% • 7%
1	C	358	% 87% 5% • 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8512 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Ornithine carbamoyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	8	0
			2610	1664	438	490	18			
1	B	333	Total	C	N	O	S	0	6	0
			2597	1653	434	492	18			
1	C	334	Total	C	N	O	S	0	6	0
			2604	1657	434	495	18			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP Q8DCF5
A	-22	HIS	-	expression tag	UNP Q8DCF5
A	-21	HIS	-	expression tag	UNP Q8DCF5
A	-20	HIS	-	expression tag	UNP Q8DCF5
A	-19	HIS	-	expression tag	UNP Q8DCF5
A	-18	HIS	-	expression tag	UNP Q8DCF5
A	-17	HIS	-	expression tag	UNP Q8DCF5
A	-16	SER	-	expression tag	UNP Q8DCF5
A	-15	SER	-	expression tag	UNP Q8DCF5
A	-14	GLY	-	expression tag	UNP Q8DCF5
A	-13	VAL	-	expression tag	UNP Q8DCF5
A	-12	ASP	-	expression tag	UNP Q8DCF5
A	-11	LEU	-	expression tag	UNP Q8DCF5
A	-10	GLY	-	expression tag	UNP Q8DCF5
A	-9	THR	-	expression tag	UNP Q8DCF5
A	-8	GLU	-	expression tag	UNP Q8DCF5
A	-7	ASN	-	expression tag	UNP Q8DCF5
A	-6	LEU	-	expression tag	UNP Q8DCF5
A	-5	TYR	-	expression tag	UNP Q8DCF5
A	-4	PHE	-	expression tag	UNP Q8DCF5
A	-3	GLN	-	expression tag	UNP Q8DCF5
A	-2	SER	-	expression tag	UNP Q8DCF5
A	-1	ASN	-	expression tag	UNP Q8DCF5

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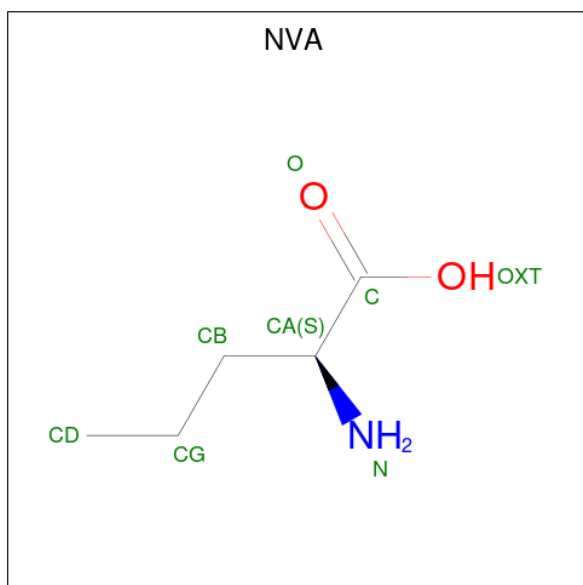
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	expression tag	UNP Q8DCF5
B	-23	MET	-	expression tag	UNP Q8DCF5
B	-22	HIS	-	expression tag	UNP Q8DCF5
B	-21	HIS	-	expression tag	UNP Q8DCF5
B	-20	HIS	-	expression tag	UNP Q8DCF5
B	-19	HIS	-	expression tag	UNP Q8DCF5
B	-18	HIS	-	expression tag	UNP Q8DCF5
B	-17	HIS	-	expression tag	UNP Q8DCF5
B	-16	SER	-	expression tag	UNP Q8DCF5
B	-15	SER	-	expression tag	UNP Q8DCF5
B	-14	GLY	-	expression tag	UNP Q8DCF5
B	-13	VAL	-	expression tag	UNP Q8DCF5
B	-12	ASP	-	expression tag	UNP Q8DCF5
B	-11	LEU	-	expression tag	UNP Q8DCF5
B	-10	GLY	-	expression tag	UNP Q8DCF5
B	-9	THR	-	expression tag	UNP Q8DCF5
B	-8	GLU	-	expression tag	UNP Q8DCF5
B	-7	ASN	-	expression tag	UNP Q8DCF5
B	-6	LEU	-	expression tag	UNP Q8DCF5
B	-5	TYR	-	expression tag	UNP Q8DCF5
B	-4	PHE	-	expression tag	UNP Q8DCF5
B	-3	GLN	-	expression tag	UNP Q8DCF5
B	-2	SER	-	expression tag	UNP Q8DCF5
B	-1	ASN	-	expression tag	UNP Q8DCF5
B	0	ALA	-	expression tag	UNP Q8DCF5
C	-23	MET	-	expression tag	UNP Q8DCF5
C	-22	HIS	-	expression tag	UNP Q8DCF5
C	-21	HIS	-	expression tag	UNP Q8DCF5
C	-20	HIS	-	expression tag	UNP Q8DCF5
C	-19	HIS	-	expression tag	UNP Q8DCF5
C	-18	HIS	-	expression tag	UNP Q8DCF5
C	-17	HIS	-	expression tag	UNP Q8DCF5
C	-16	SER	-	expression tag	UNP Q8DCF5
C	-15	SER	-	expression tag	UNP Q8DCF5
C	-14	GLY	-	expression tag	UNP Q8DCF5
C	-13	VAL	-	expression tag	UNP Q8DCF5
C	-12	ASP	-	expression tag	UNP Q8DCF5
C	-11	LEU	-	expression tag	UNP Q8DCF5
C	-10	GLY	-	expression tag	UNP Q8DCF5
C	-9	THR	-	expression tag	UNP Q8DCF5
C	-8	GLU	-	expression tag	UNP Q8DCF5
C	-7	ASN	-	expression tag	UNP Q8DCF5

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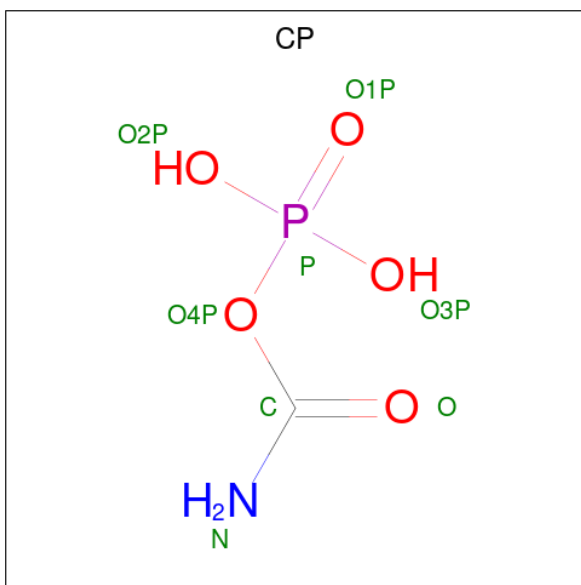
Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	LEU	-	expression tag	UNP Q8DCF5
C	-5	TYR	-	expression tag	UNP Q8DCF5
C	-4	PHE	-	expression tag	UNP Q8DCF5
C	-3	GLN	-	expression tag	UNP Q8DCF5
C	-2	SER	-	expression tag	UNP Q8DCF5
C	-1	ASN	-	expression tag	UNP Q8DCF5
C	0	ALA	-	expression tag	UNP Q8DCF5

- Molecule 2 is NORVALINE (CCD ID: NVA) (formula: $C_5H_{11}NO_2$).



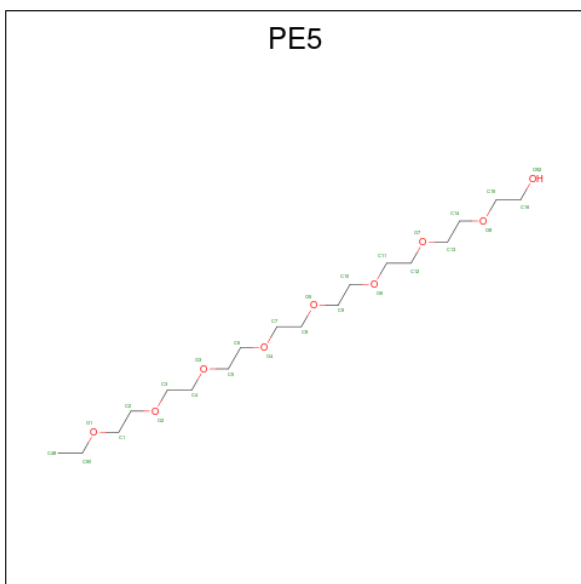
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			8	5	1	2		
2	B	1	Total	C	N	O	0	0
			8	5	1	2		
2	C	1	Total	C	N	O	0	0
			8	5	1	2		

- Molecule 3 is PHOSPHORIC ACID MONO(FORMAMIDE)ESTER (CCD ID: CP) (formula: CH_4NO_5P).



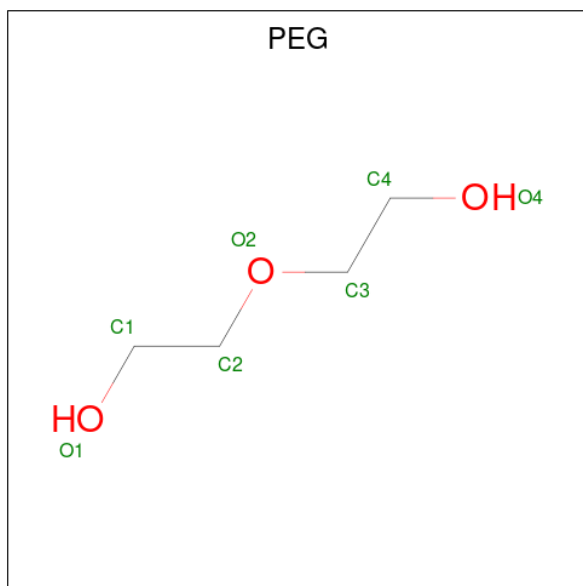
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 8	C 1	N 1	O 5	P 1	0	0
3	B	1	Total 8	C 1	N 1	O 5	P 1	0	0
3	C	1	Total 8	C 1	N 1	O 5	P 1	0	0

- Molecule 4 is 3,6,9,12,15,18,21,24-OCTAOXAHEXACOSAN-1-OL (CCD ID: PE5) (formula: $\text{C}_{18}\text{H}_{38}\text{O}_9$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			16	10	6		
4	B	1	Total	C	O	0	0
			10	6	4		
4	C	1	Total	C	O	0	0
			11	7	4		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 6 4 2	0	0
5	B	1	Total C O 5 3 2	0	0
5	C	1	Total C O 5 3 2	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Cl 2 2	0	0
6	B	2	Total Cl 2 2	0	0
6	C	2	Total Cl 2 2	0	0

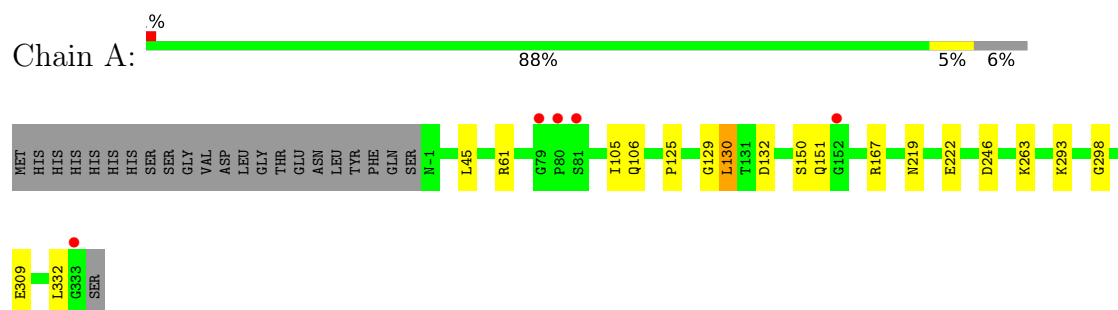
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	194	Total O 194 194	0	0
7	B	161	Total O 161 161	0	0
7	C	140	Total O 140 140	0	1

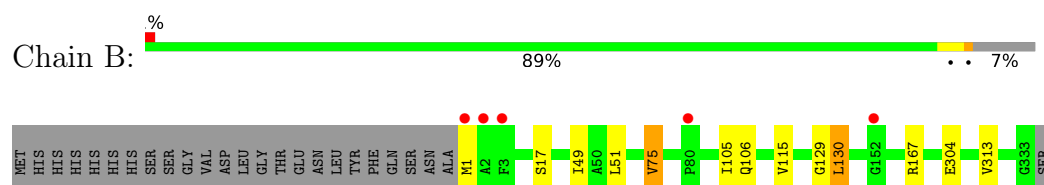
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

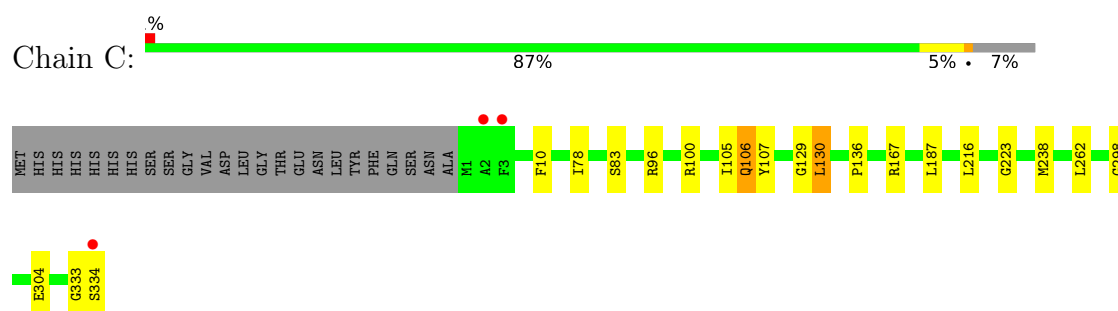
- Molecule 1: Ornithine carbamoyltransferase



- Molecule 1: Ornithine carbamoyltransferase



- Molecule 1: Ornithine carbamoyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.26Å 80.91Å 152.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.70 50.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-1.70) 100.0 (50.00-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.135 , 0.167 0.149 , 0.175	Depositor DCC
R_{free} test set	5135 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	21.1	Xtriage
Anisotropy	0.166	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	8512	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PE5, CL, NVA, CP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.15	3/2684 (0.1%)	1.02	0/3626
1	B	1.03	1/2662 (0.0%)	0.97	1/3596 (0.0%)
1	C	1.03	4/2670 (0.1%)	0.98	0/3607
All	All	1.07	8/8016 (0.1%)	0.99	1/10829 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	ILE	C-O	-7.14	1.16	1.24
1	C	105	ILE	C-O	-6.52	1.17	1.24
1	A	61	ARG	C-O	-6.47	1.16	1.24
1	A	298	GLY	N-CA	5.64	1.51	1.45
1	C	106	GLN	C-O	-5.57	1.17	1.23
1	B	105	ILE	C-O	-5.51	1.18	1.24
1	C	107	TYR	C-O	-5.10	1.18	1.24
1	C	223	GLY	C-O	-5.00	1.18	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	313	VAL	N-CA-C	5.30	117.67	111.05

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2610	0	2597	10	0
1	B	2597	0	2584	12	0
1	C	2604	0	2572	10	0
2	A	8	0	10	0	0
2	B	8	0	10	0	0
2	C	8	0	10	0	0
3	A	8	0	2	0	0
3	B	8	0	2	0	0
3	C	8	0	2	0	0
4	A	16	0	20	0	0
4	B	10	0	12	0	0
4	C	11	0	12	1	0
5	A	53	0	75	2	0
5	B	36	0	47	1	0
5	C	26	0	35	2	0
6	A	2	0	0	0	0
6	B	2	0	0	1	0
6	C	2	0	0	1	0
7	A	194	0	0	0	0
7	B	161	0	0	0	0
7	C	140	0	0	1	0
All	All	8512	0	7990	33	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (33) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:N	1:B:1:MET:HE2	2.09	0.68
1:C:187[A]:LEU:HD12	1:C:216:LEU:CD2	2.32	0.60
1:B:49[B]:ILE:CG1	1:B:75[B]:VAL:HG22	2.33	0.58
1:C:238:MET:HA	5:C:409:PEG:H41	1.86	0.57
1:B:49[B]:ILE:HG13	1:B:75[B]:VAL:HG22	1.88	0.54
1:C:130:LEU:HD23	1:C:130:LEU:C	2.33	0.54
1:B:51:LEU:CD1	1:B:75[B]:VAL:HG11	2.38	0.54
1:B:1:MET:HE2	1:B:1:MET:H3	1.73	0.53
1:B:1:MET:HE2	1:B:1:MET:H1	1.75	0.52
1:C:333:GLY:O	1:C:334:SER:C	2.53	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:GLU:H	1:A:309:GLU:CD	2.18	0.50
1:A:246:ASP:OD1	1:A:293:LYS:NZ	2.32	0.49
1:B:130:LEU:C	1:B:130:LEU:HD23	2.38	0.48
1:A:132:ASP:HB3	5:A:405:PEG:H31	1.94	0.48
1:B:129:GLY:O	1:B:130:LEU:CB	2.62	0.47
1:A:130:LEU:C	1:A:130:LEU:HD23	2.40	0.47
1:C:304[B]:GLU:OE1	6:C:408:CL:CL	2.70	0.47
1:B:17:SER:HA	5:B:411:PEG:H11	1.97	0.47
1:A:219[B]:ASN:HB3	1:A:222:GLU:HG2	1.97	0.46
1:B:49[B]:ILE:HD12	1:B:51:LEU:HD21	1.98	0.46
1:B:51:LEU:HD11	1:B:75[B]:VAL:HG11	1.98	0.45
1:C:10:PHE:CE2	1:C:136:PRO:HB2	2.51	0.45
1:C:129:GLY:O	1:C:130:LEU:CB	2.65	0.45
1:A:129:GLY:O	1:A:130:LEU:CB	2.65	0.44
4:C:404:PE5:H31	7:C:526:HOH:O	2.17	0.44
1:A:263:LYS:HA	5:A:406:PEG:H31	2.00	0.44
1:C:262:LEU:HB3	5:C:406:PEG:H32	2.00	0.43
1:A:45[B]:LEU:HD23	1:A:45[B]:LEU:HA	1.81	0.43
1:C:78:ILE:HG23	1:C:83:SER:HB3	2.03	0.41
1:A:150:SER:O	1:A:151:GLN:HG2	2.20	0.41
1:B:304:GLU:OE1	6:B:406:CL:CL	2.76	0.40
1:A:125:PRO:HG2	1:A:332[A]:LEU:HD23	2.04	0.40
1:C:96:ARG:O	1:C:100:ARG:HG2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	341/358 (95%)	334 (98%)	6 (2%)	1 (0%)	36	22
1	B	337/358 (94%)	330 (98%)	6 (2%)	1 (0%)	36	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	338/358 (94%)	329 (97%)	7 (2%)	2 (1%)	21	9
All	All	1016/1074 (95%)	993 (98%)	19 (2%)	4 (0%)	30	16

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	130	LEU
1	B	130	LEU
1	C	130	LEU
1	C	298	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	273/292 (94%)	271 (99%)	2 (1%)	76	69
1	B	273/292 (94%)	268 (98%)	5 (2%)	51	36
1	C	272/292 (93%)	270 (99%)	2 (1%)	76	69
All	All	818/876 (93%)	809 (99%)	9 (1%)	68	54

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	GLN
1	A	167	ARG
1	B	75[A]	VAL
1	B	75[B]	VAL
1	B	106	GLN
1	B	115	VAL
1	B	167	ARG
1	C	106	GLN
1	C	167	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such

sidechains are listed below:

Mol	Chain	Res	Type
1	B	264	GLN
1	C	159	GLN
1	C	172	ASN
1	C	256	GLN
1	C	258	ASN
1	C	269	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 6 are monoatomic - leaving 27 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CP	B	402	-	6,7,7	2.23	2 (33%)	7,10,10	1.46	1 (14%)
4	PE5	C	404	-	10,10,26	0.55	0	9,9,25	0.46	0
5	PEG	C	406	-	6,6,6	0.47	0	5,5,5	0.93	0
5	PEG	A	406	-	6,6,6	0.22	0	5,5,5	0.65	0
5	PEG	A	404	-	6,6,6	0.67	0	5,5,5	0.38	0
5	PEG	C	409	-	6,6,6	0.40	0	5,5,5	1.13	0
5	PEG	A	409	-	6,6,6	0.44	0	5,5,5	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PE5	A	403	-	15,15,26	0.43	0	14,14,25	0.49	0
5	PEG	C	405	-	4,4,6	0.44	0	3,3,5	0.20	0
2	NVA	B	401	-	6,7,7	1.18	1 (16%)	5,8,8	0.88	0
4	PE5	B	410	-	9,9,26	0.46	0	8,8,25	0.69	0
2	NVA	A	401	-	6,7,7	0.80	0	5,8,8	0.70	0
5	PEG	A	408	-	6,6,6	0.38	0	5,5,5	0.32	0
5	PEG	B	405	-	6,6,6	0.35	0	5,5,5	0.29	0
5	PEG	B	409	-	5,5,6	0.87	0	4,4,5	1.30	1 (25%)
5	PEG	B	408	-	3,3,6	0.62	0	2,2,5	0.18	0
5	PEG	A	410	-	3,3,6	0.53	0	2,2,5	0.39	0
3	CP	A	402	-	6,7,7	1.20	1 (16%)	7,10,10	0.93	0
5	PEG	C	407	-	6,6,6	0.59	0	5,5,5	0.85	0
5	PEG	A	405	-	6,6,6	0.58	0	5,5,5	1.09	1 (20%)
5	PEG	B	407	-	6,6,6	0.53	0	5,5,5	0.28	0
5	PEG	A	413	-	6,6,6	0.54	0	5,5,5	0.21	0
5	PEG	B	411	-	4,4,6	0.65	0	3,3,5	0.46	0
2	NVA	C	401	-	6,7,7	0.83	0	5,8,8	0.33	0
3	CP	C	403	-	6,7,7	2.31	1 (16%)	7,10,10	1.56	2 (28%)
5	PEG	B	403	-	6,6,6	0.31	0	5,5,5	0.29	0
5	PEG	A	412	-	6,6,6	0.68	0	5,5,5	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	CP	B	402	-	-	0/3/5/5	-
4	PE5	C	404	-	-	2/8/8/24	-
5	PEG	C	406	-	-	2/4/4/4	-
5	PEG	A	406	-	-	3/4/4/4	-
5	PEG	A	404	-	-	2/4/4/4	-
5	PEG	C	409	-	-	3/4/4/4	-
5	PEG	A	409	-	-	1/4/4/4	-
4	PE5	A	403	-	-	3/13/13/24	-
5	PEG	C	405	-	-	2/2/2/4	-
2	NVA	B	401	-	-	1/7/7/7	-
4	PE5	B	410	-	-	3/7/7/24	-
2	NVA	A	401	-	-	2/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	408	-	-	3/4/4/4	-
5	PEG	B	405	-	-	2/4/4/4	-
5	PEG	B	409	-	-	1/3/3/4	-
5	PEG	B	408	-	-	1/1/1/4	-
5	PEG	A	410	-	-	1/1/1/4	-
3	CP	A	402	-	-	0/3/5/5	-
5	PEG	C	407	-	-	3/4/4/4	-
5	PEG	A	405	-	-	3/4/4/4	-
5	PEG	B	407	-	-	0/4/4/4	-
5	PEG	A	413	-	-	3/4/4/4	-
5	PEG	B	411	-	-	2/2/2/4	-
2	NVA	C	401	-	-	2/7/7/7	-
3	CP	C	403	-	-	0/3/5/5	-
5	PEG	B	403	-	-	1/4/4/4	-
5	PEG	A	412	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	CP	P-O4P	4.83	1.68	1.59
3	B	402	CP	P-O4P	4.45	1.67	1.59
3	B	402	CP	P-O3P	-2.79	1.44	1.54
3	A	402	CP	O-C	2.64	1.26	1.22
2	B	401	NVA	OXT-C	-2.01	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	CP	O3P-P-O2P	2.63	117.65	107.80
3	B	402	CP	O3P-P-O2P	2.36	116.64	107.80
5	B	409	PEG	C3-O2-C2	2.33	121.22	113.06
3	C	403	CP	O3P-P-O4P	-2.32	98.57	105.32
5	A	405	PEG	O2-C3-C4	2.05	119.16	110.11

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	409	PEG	C1-C2-O2-C3
5	B	405	PEG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
5	A	406	PEG	O1-C1-C2-O2
5	A	408	PEG	O2-C3-C4-O4
5	A	404	PEG	O1-C1-C2-O2
4	A	403	PE5	O6-C10-C9-O5
5	C	405	PEG	O1-C1-C2-O2
5	C	407	PEG	O2-C3-C4-O4
5	B	403	PEG	O1-C1-C2-O2
5	A	406	PEG	O2-C3-C4-O4
5	A	413	PEG	O2-C3-C4-O4
5	B	411	PEG	O1-C1-C2-O2
5	C	407	PEG	C1-C2-O2-C3
4	C	404	PE5	O3-C5-C6-O4
5	A	413	PEG	C1-C2-O2-C3
5	A	404	PEG	C1-C2-O2-C3
5	C	409	PEG	C1-C2-O2-C3
5	A	409	PEG	C4-C3-O2-C2
5	A	406	PEG	C1-C2-O2-C3
5	C	406	PEG	C1-C2-O2-C3
4	C	404	PE5	C5-C6-O4-C7
5	B	405	PEG	O2-C3-C4-O4
5	C	409	PEG	O2-C3-C4-O4
4	B	410	PE5	O3-C5-C6-O4
5	A	405	PEG	O2-C3-C4-O4
5	C	406	PEG	O2-C3-C4-O4
5	A	408	PEG	C4-C3-O2-C2
5	A	413	PEG	O1-C1-C2-O2
2	A	401	NVA	OXT-C-CA-N
4	B	410	PE5	O1-C1-C2-O2
2	B	401	NVA	OXT-C-CA-N
2	C	401	NVA	OXT-C-CA-N
5	B	411	PEG	C1-C2-O2-C3
5	A	405	PEG	C1-C2-O2-C3
4	B	410	PE5	C1-C2-O2-C3
2	C	401	NVA	O-C-CA-N
5	A	410	PEG	O2-C3-C4-O4
5	B	408	PEG	O1-C1-C2-O2
5	C	405	PEG	C1-C2-O2-C3
4	A	403	PE5	O2-C3-C4-O3
5	A	405	PEG	O1-C1-C2-O2
5	A	408	PEG	C1-C2-O2-C3
4	A	403	PE5	C5-C6-O4-C7
5	C	407	PEG	O1-C1-C2-O2

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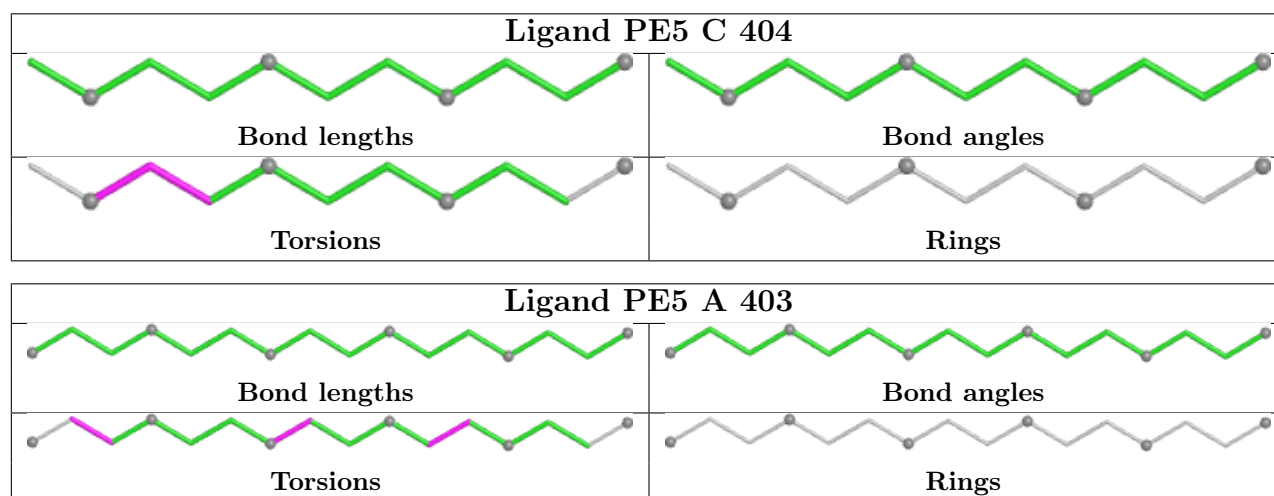
Mol	Chain	Res	Type	Atoms
5	C	409	PEG	C4-C3-O2-C2
2	A	401	NVA	O-C-CA-N

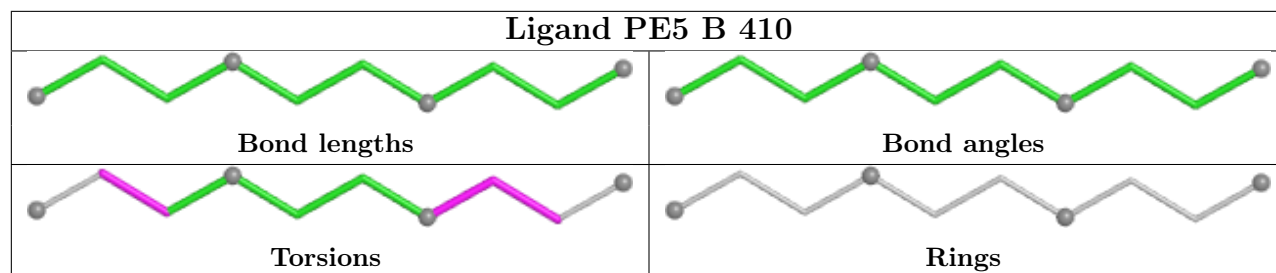
There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	404	PE5	1	0
5	C	406	PEG	1	0
5	A	406	PEG	1	0
5	C	409	PEG	1	0
5	A	405	PEG	1	0
5	B	411	PEG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/358 (93%)	-0.37	5 (1%) 72 76	10, 19, 34, 53	8 (2%)
1	B	333/358 (93%)	-0.24	5 (1%) 72 76	11, 23, 41, 88	6 (1%)
1	C	334/358 (93%)	-0.22	3 (0%) 81 83	11, 24, 41, 76	6 (1%)
All	All	1002/1074 (93%)	-0.28	13 (1%) 75 79	10, 22, 40, 88	20 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	80	PRO	5.4
1	B	3	PHE	5.4
1	B	2	ALA	4.2
1	B	1	MET	3.2
1	C	2	ALA	3.1
1	C	3	PHE	3.1
1	A	79	GLY	2.8
1	A	333	GLY	2.4
1	A	81	SER	2.4
1	B	152	GLY	2.4
1	B	80	PRO	2.2
1	C	334	SER	2.2
1	A	152	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

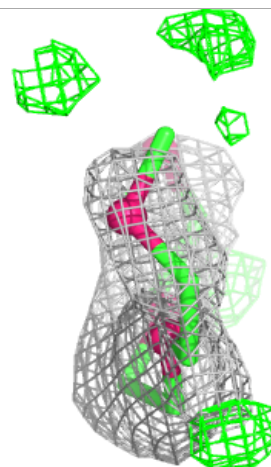
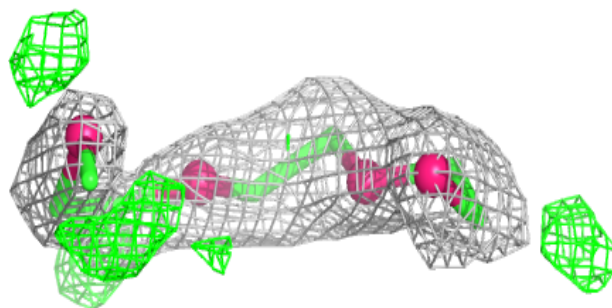
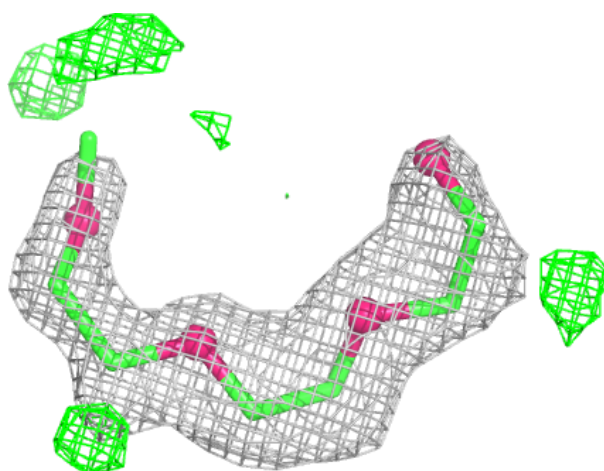
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	PEG	C	409	7/7	0.61	0.18	41,45,48,50	0
5	PEG	B	408	4/7	0.66	0.19	47,48,52,55	0
5	PEG	B	409	6/7	0.68	0.18	37,42,46,47	0
5	PEG	C	405	5/7	0.74	0.21	53,54,55,63	0
4	PE5	C	404	11/27	0.74	0.16	42,48,62,65	0
5	PEG	A	404	7/7	0.75	0.15	38,40,44,46	0
5	PEG	A	413	7/7	0.75	0.15	52,57,62,63	0
5	PEG	A	410	4/7	0.76	0.16	41,42,44,50	0
5	PEG	A	405	7/7	0.78	0.14	36,39,42,49	0
5	PEG	A	412	7/7	0.79	0.14	41,49,55,56	0
5	PEG	C	407	7/7	0.82	0.16	51,52,55,56	0
5	PEG	B	407	7/7	0.83	0.14	51,52,60,60	0
5	PEG	B	403	7/7	0.83	0.14	48,50,54,56	0
5	PEG	B	411	5/7	0.84	0.12	32,32,41,48	0
5	PEG	A	406	7/7	0.85	0.15	38,41,48,49	0
4	PE5	A	403	16/27	0.85	0.13	36,54,61,62	0
5	PEG	B	405	7/7	0.88	0.12	49,51,56,56	0
5	PEG	A	408	7/7	0.88	0.12	52,55,56,65	0
5	PEG	C	406	7/7	0.90	0.11	36,41,48,49	0
4	PE5	B	410	10/27	0.90	0.11	34,41,47,52	0
5	PEG	A	409	7/7	0.90	0.11	38,42,45,50	0
2	NVA	C	401	8/8	0.96	0.06	17,19,19,20	0
2	NVA	B	401	8/8	0.96	0.06	19,20,21,21	0
2	NVA	A	401	8/8	0.97	0.04	15,17,18,19	0
6	CL	B	406	1/1	0.97	0.16	41,41,41,41	0
6	CL	C	408	1/1	0.98	0.07	36,36,36,36	0
3	CP	C	403	8/8	0.99	0.04	15,15,18,18	0
6	CL	A	407	1/1	0.99	0.02	16,16,16,16	0
6	CL	A	411	1/1	0.99	0.04	30,30,30,30	0
6	CL	B	404	1/1	0.99	0.04	19,19,19,19	0
3	CP	A	402	8/8	0.99	0.04	15,16,18,19	0
6	CL	C	402	1/1	0.99	0.04	21,21,21,21	0
3	CP	B	402	8/8	0.99	0.04	16,17,21,21	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

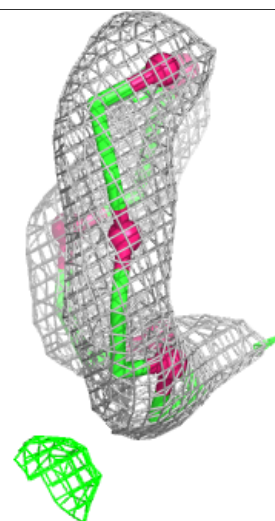
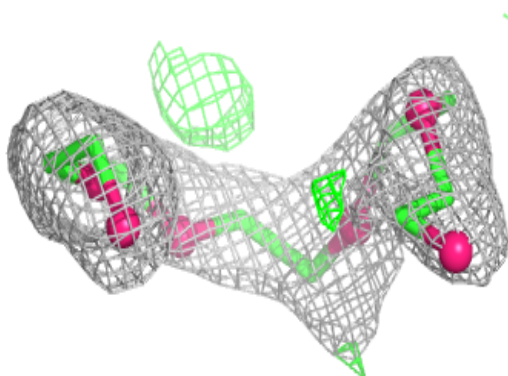
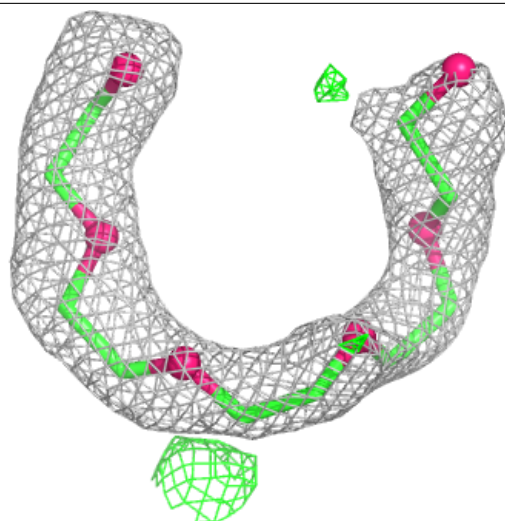
Electron density around PE5 C 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



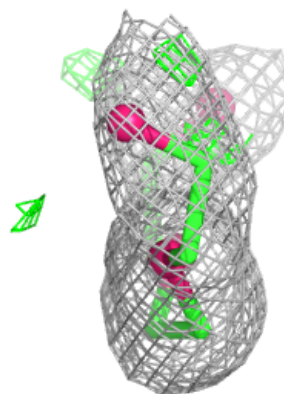
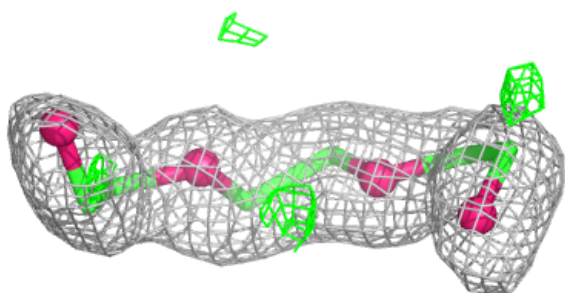
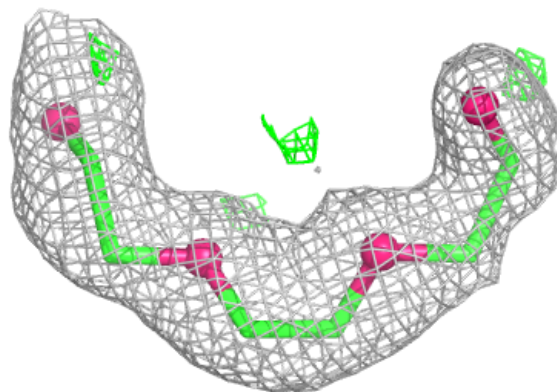
Electron density around PE5 A 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PE5 B 410:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.